

ANSWERS: Reaction schemes

1)

<p>A = Propan-2-ol</p> $\begin{array}{c} \text{OH} \\ \\ \text{CH}_3\text{CHCH}_3 \end{array}$ <p>B = Propan-1-ol</p> $\text{CH}_3\text{CH}_2\text{CH}_2\text{OH}$ <p>C = Propanone</p> $\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{CCH}_3 \end{array}$	<p>D = Propanoic acid</p> $\text{CH}_3\text{CH}_2\text{COOH}$ <p>E = Propanoyl chloride</p> $\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{CH}_2\text{CCl} \end{array}$ <p>F = Propanamide</p> $\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{CH}_2\text{C} \\ \backslash \\ \text{NH}_2 \end{array}$	<p>G = Propyl propanoate</p> $\begin{array}{c} \text{O} \\ \\ \text{CH}_3\text{CH}_2\text{C} \end{array} \text{OCH}_2\text{CH}_2\text{CH}_3$ <p>H = Methyl ethyl propanoate (not required)</p> $\text{CH}_3\text{CH}_2 - \begin{array}{c} \text{O} \\ \\ \text{C} \end{array} - \text{O} - \begin{array}{c} \text{CH}_3 \\ \\ \text{CH} \end{array} \text{CH}_3$
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2)

Reagent: NaBH_4 / LiAlH_4

Type of reaction – reduction / redox

Reagent: conc H_2SO_4 / conc H_3PO_4 / Al_2O_3

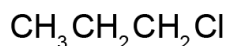
Type of reaction – elimination / dehydration / condensation

Explanation:

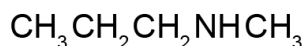
- An elimination reaction occurs because the molecule has changed from saturated to unsaturated / a ($\text{C}=\text{C}$) double bond forms.
 - Because water is removed / H and OH have been removed (from adjacent C atoms).
 - The but-2-ene is the major product / but-1-ene is the minor product.
 - A mixture of products is formed, because the two carbons adjacent to the carbon-bearing OH have different numbers of H atoms attached / it is asymmetric.
- (Zaitsev's rule – the major product has the more substituted double bond)

3) 1 SOCl_2 (Accept PCl_3 , PCl_5 or conc HCl / ZnCl_2)

B

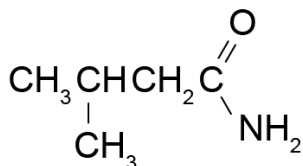


C



4) Name: 3 methyl butanoyl chloride.

Products:



Hydrogen chloride / HCl / ammonium chloride / NH_4Cl

5) NaOH or KOH (alcoholic)

Elimination reaction

This is an elimination reaction as a hydrogen atom and a chlorine atom on adjacent carbon atoms are removed, forming a carbon-to-carbon double bond.

6)

<p>a) Product A:</p> $\begin{array}{c} \text{H} & \text{H} & \text{H} & \text{O} \\ & & & // \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C} \\ & & & \backslash \\ \text{H} & \text{H} & \text{H} & \text{O}-\text{H} \end{array}$ <p>butanoic acid</p> <p>Product B:</p> $\begin{array}{c} \text{H} & \text{H} & \text{H} & \text{H} & \text{O} \\ & & & & // \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C}-\text{C} \\ & & & & \backslash \\ \text{H} & \text{H} & \text{H} & \text{H} & \text{H} \end{array}$ <p>butan-1-ol</p>	<p>Product C:</p> $\begin{array}{c} & \text{H} & \text{H} & \text{H} \\ & & & \\ \text{H} & \text{C}=\text{C} & -\text{C} & -\text{C}-\text{H} \\ & & & \\ & \text{H} & \text{H} & \text{H} \end{array}$ <p>but-1-ene</p>
<p>b) Reactant 1 → no reaction</p> <p>Reactant 2 → butan-2-ol</p>	<p>Reactant 3 →</p> $\begin{array}{c} & & \text{H} & & \\ & & & & \\ \text{H} & \text{H} & \text{O} & \text{H} \\ & & & \\ \text{H}-\text{C}-\text{C}-\text{C}-\text{C}-\text{H} \\ & & & \\ \text{H} & \text{H} & \text{H} & \text{H} \end{array}$
<p>major product</p> $\begin{array}{c} & \text{H} & & \text{H} \\ & & & \\ \text{H} & \text{C}=\text{C} & & \text{H} \\ & & & \\ \text{H} & \text{C} & & \text{H} \\ & & & \\ \text{H} & & & \text{H} \end{array}$ <p>but-2-ene</p>	<p>minor product</p> $\begin{array}{c} & \text{H} & \text{H} & \text{H} \\ & & & \\ \text{H} & \text{C}=\text{C} & -\text{C} & -\text{C}-\text{H} \\ & & & \\ \text{H} & & \text{H} & \text{H} \end{array}$ <p>but-1-ene</p>

c) Butanal /aldehydes can be oxidised using $\text{Cr}_2\text{O}_7^{2-}/\text{H}^+$ (Reactant 1) to form a carboxylic acid, butanoic acid. However, butanone/ketones cannot be oxidised.

Both butanal/aldehydes and butanone/ketones can be reduced using NaBH_4 (Reactant 2) to form alcohols.

Aldehydes form primary alcohols and ketones form secondary alcohols.

With concentrated H_2SO_4 alcohols form alkenes.

The primary alcohol $\text{CH}_3-\text{CH}_2-\text{CH}_2-\text{CH}_2\text{OH}$ forms only one product as the H and OH atoms on adjacent carbon atoms are replaced with a carbon-to-carbon double bond.

The secondary alcohol $\text{CH}_3-\text{CH}_2-\text{CHOH}-\text{CH}_3$ forms a mixture of products as OH is on the 2nd carbon atom. Either the 1st H is removed, forming

$\text{CH}_3-\text{CH}_2-\text{CH}=\text{CH}_2$ (minor) or the 3rd H is removed, forming $\text{CH}_3-\text{CH}=\text{CH}-\text{CH}_3$ (major).

7)

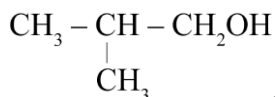
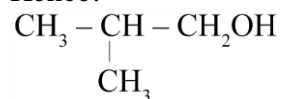
W	$\begin{array}{c} \text{CH}_3-\text{CH}-\text{CH}_2\text{OH} \\ \\ \text{CH}_3 \end{array}$	Y	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3-\text{CH}-\text{C}-\text{Cl} \\ \\ \text{CH}_3 \end{array}$
X	$\begin{array}{c} \text{O} \\ \\ \text{CH}_3-\text{CH}-\text{C}-\text{OH} \\ \\ \text{CH}_3 \end{array}$	Z	$\begin{array}{c} \text{O} & \text{H} \\ & \\ \text{CH}_3-\text{CH}-\text{C}-\text{NCH}_3 \\ \\ \text{CH}_3 \end{array}$

Compound W

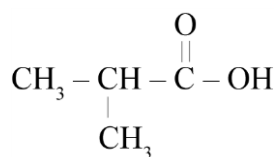
This compound is oxidised by $\text{Cr}_2\text{O}_7^{2-}/\text{H}^+$ to an acid so it has to be a primary alcohol (or an aldehyde –

rejected as too many H atoms). The OH has to be on an end C. It's a branched chain molecule so there is a CH₃ on the 2nd C atom.

Hence:



Compound X This is formed when is oxidised to an acid. Hence:

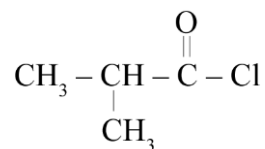


Compound Y

A substitution reaction occurs with SOCl₂; the OH in

is replaced with Cl.

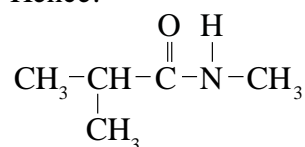
Hence:



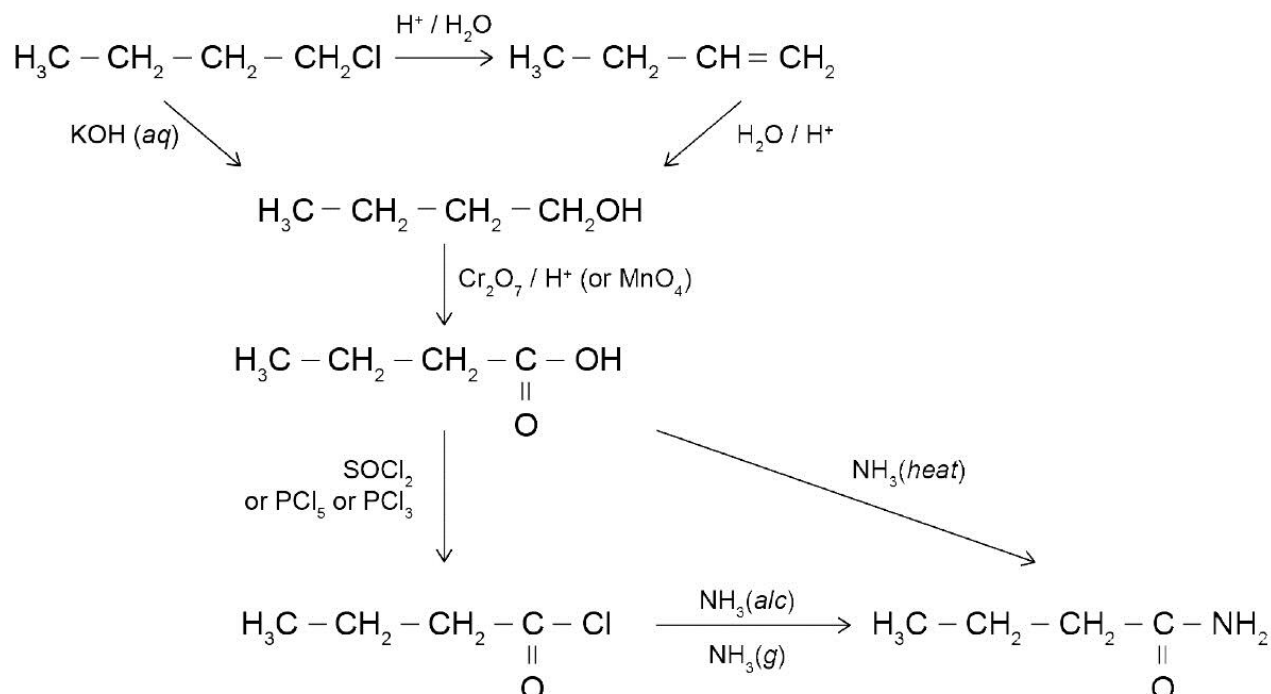
Compound Z

A substitution reaction occurs with CH₃NH₂; the Cl is replaced with CH₃NH₂.

Hence:

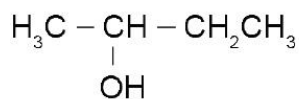


8)

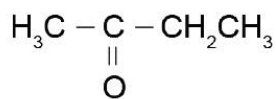


9)

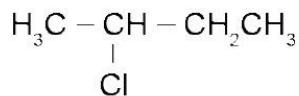
A (butan-2-ol)



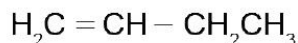
B (butanone)



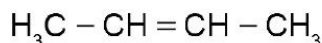
C (2-chlorobutane)



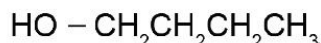
D (but-1-ene)



E (but-2-ene)



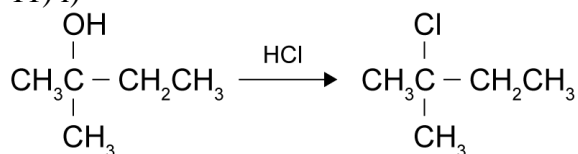
F (butan-1-ol)



10)

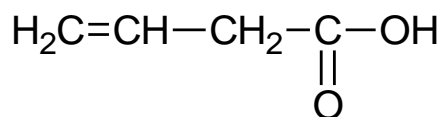
<p>A</p> $\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C}-\text{CH}_2-\text{C} \\ \\ \text{O}-\text{CH}_2-\text{CH}_2-\text{CH}_3 \end{array}$ <p>propyl propanoate</p> <p>B - sodium propanoate</p> <p>C</p> $\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{OH}$ <p>propan-1ol (1-propanol)</p> <p>D</p> $\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C}-\text{CH}_2-\text{C} \\ \\ \text{OH} \end{array} \quad \text{OR} \quad \begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C}-\text{CH}_2-\text{C} \\ \\ \text{Cl} \end{array}$ <p>propanoic acid propanoyl chloride</p> <p>OR methylpropanoate</p> <p>E</p> $\begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C}-\text{CH}_2-\text{C} \\ \\ \text{H} \end{array} \quad \text{OR} \quad \begin{array}{c} \text{O} \\ \\ \text{H}_3\text{C}-\text{CH}_2-\text{C} \\ \\ \text{OH} \end{array}$ <p>propanal propanoic acid</p> <p>F</p> $\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2\text{Cl}$	<p>Reagent 1 = NaOH(aq)</p> <p>Reagent 2 = NaOH(aq), <i>accept NaOH(alc) if D = acid chloride, Na₂CO₃ (aq).</i></p> <p>Reagent 3 = PCl₅ / SOCl₂ / PCl₃.</p> <p>Reagent 4 = Cr₂O₇²⁻ / H⁺ or MnO₄⁻ / (H⁺) / Fehling / Benedicts/ Tollens <i>or if D is given as acid chloride, accept PCl₅ / SOCl₂ / PCl₃ / methanol or other alcohol + acid to give ester in D.</i></p>
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11) i)

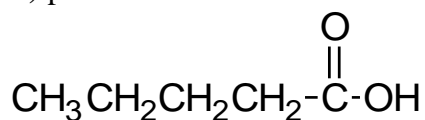


ii) Substitution, the alcohol group is removed and substituted with the chlorine side chain

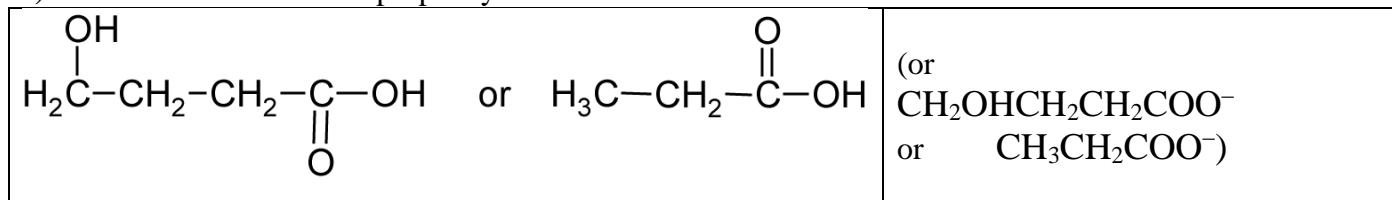
12) i) 4-chlorobutanoic acid



ii) pentanal



iii) 4-chlorobutanoic acid or propanoyl chloride



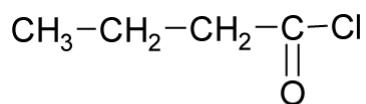
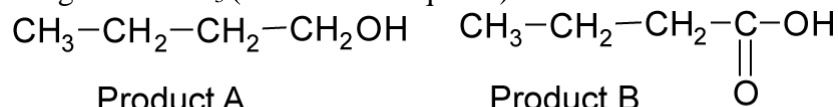
13)

Reagent 1 $\text{H}^+ / \text{Cr}_2\text{O}_7^{2-}$ OR $\text{MnO}_4^- / \text{H}^+$ OR MnO_4^-

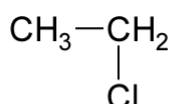
Reagent 2 $\text{PCl}_3 / \text{PCl}_5 / \text{SOCl}_2$ OR HBr OR SOBr_2

Reagent 3 $\text{PCl}_3 / \text{PCl}_5 / \text{SOCl}_2$ / conc HCl with ZnCl_2 (not just conc HCl)

Reagent 4 NH_3 (alcohol not required)



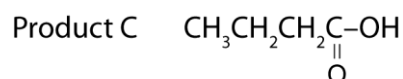
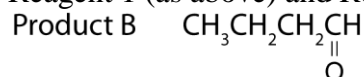
Product C



Product D

Alternative answer:

Reagent 1 (as above) and Reagent 2 = Reagent 1 OR Tollens / Benedicts / Fehlings



14) Aldehyde (propanal) is obtained by heating a mixture of propan-1-ol with acidified (potassium dichromate) solution or (acidified) permanganate solution. Propanal can be removed from the solution as it forms, using distillation, as the aldehyde has a lower boiling point than propan-1-ol and the carboxylic acid. Carboxylic acid (propanoic acid) is obtained by reacting a mixture of propan-1-ol with acidified potassium dichromate solution (under reflux conditions) until all of the reactant has been converted to propanoic acid.

15)

Reagent	Formula
1	PCl_3 , or PCl_5 , or SOCl_2 , or HCl
2	NH_3
3	$\text{Cr}_2\text{O}_7^{2-} / \text{H}^+$ or $\text{MnO}_4^- / \text{H}^+$
4	PCl_3 , or PCl_5 , or SOCl_2
5	CH_3NH_2

16)

Product	Name or formula
1	$\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{Cl}$
2	$\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{C} \begin{smallmatrix} \text{O} \\ // \\ \text{OH} \end{smallmatrix}$
3	$\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{C} \begin{smallmatrix} \text{O} \\ // \\ \text{Cl} \end{smallmatrix}$

Product	Name or formula
1	$\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{Cl}$
2	$\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{C} \begin{smallmatrix} \text{O} \\ // \\ \text{OH} \end{smallmatrix}$
3	$\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{C} \begin{smallmatrix} \text{O} \\ // \\ \text{H} \end{smallmatrix}$

17) i) SOCl_2 / PCl_3 / PCl_5 NOT HCl ii) $\text{CH}_3\text{CH}_2\text{CH}(\text{NH}_2)\text{CH}_3$

Accept recognition that substitution will not occur under these conditions alone.

iii) Reagent 1 $\text{Cr}_2\text{O}_7^{2-} / \text{H}^+$ or $\text{MnO}_4^- / \text{H}^+$ Product CH_3COOH Reagent 2 NaOH , Na_2CO_3 , NaHCO_3 iv) Reagent 1 conc H_2SO_4 Product $\text{CH}_3\text{CH}=\text{CH}_2$ Reagent 2 Dilute H_2SO_4 or $\text{H}^+ / \text{H}_2\text{O}$

18)

Reaction	Type	Reagent
1	Elimination / Dehydration	conc H_2SO_4
2	Oxidation	$\text{Cr}_2\text{O}_7^{2-} / \text{H}^+$ or $\text{MnO}_4^- / \text{H}^+$
3	Substitution	SOCl_2 , PCl_3 , PCl_5 , conc HCl

19) Reagent 1 – **KOH** in **ethanol**/alcoholReagent 2 – $\text{NaOH}(\text{aq})$ / NaOH/KOH / $\text{KOH}(\text{aq})$ / H_2O with OH^- – *not* H_2O Reagent 3 – SOCl_2 / PCl_3 / PCl_5 – *not* HCl

Compound X (Minor product): $\text{CH}_3\text{CH}_2\text{CH}_2\text{Br}$ or full structure Name of minor product: 1-bromopropane $\text{CH}_3\text{CH}_2\text{COCl}$ is propanoyl chloride	Compound Y $\text{CH}_3-\text{CH}_2-\text{C} \begin{smallmatrix} \text{O} \\ // \\ \text{O}-\text{CH}_2-\text{CH}_3 \end{smallmatrix}$ OR $\text{CH}_3\text{CH}_2\text{COOCH}_2\text{CH}_3$ or full structure Name: ethyl propanoate
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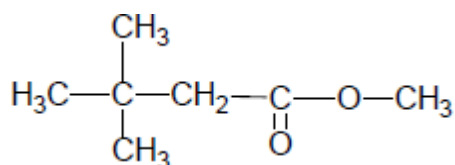
b)

(i) Elimination	The molecule HCl / a Cl atom and an H atom removed and a double bond is created.
(ii) Substitution	Br ⁻ / Br ₂ is removed and replaced / exchanged / swapped with / changed for / substituted with; an OH ⁻ / OH group.
(iii) Oxidation	Oxygen is added / hydrogen is removed / electrons are lost / the number of bonds to oxygen is increased / the oxidation number of carbon increases / Cr ₂ O ₇ ²⁻ is an oxidising agent / Cr ₂ O ₇ ²⁻ is reduced to Cr ³⁺ so the alcohol is oxidised.

c) If the major product (2-bromopropane) remains in the flask when reagent 2 (NaOH(aq)) is added, a substitution reaction would cause the formation of the 2° alcohol propan-2-ol (CH₃CH(OH)CH₃) as well as propan-1-ol. This would in turn be oxidised by the dichromate to the ketone/ propanone/ (CH₃COCH₃). No further reaction with reagent 3 or ethanol will occur, so the final mixture would contain a lot of propanone and a smaller amount of the ester.

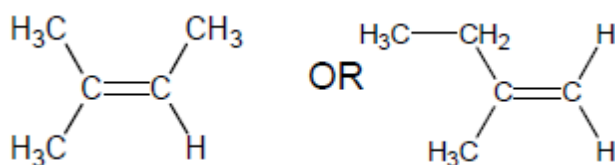
(If all of the alcohol was not completely oxidised to the ketone, an ester with the ester group attached at the 2nd C atom might form with the propanoic acid and 2-chloropropane might result from excess propan-2-ol reacting with reagent 3.)

20)



condensation /esterification/substitution

ii)



elimination